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Hyperspectral Gas Analysis System (HyGAS) SBIR Phase I Final Report

SETS Technology, Inc.
300 Kahelu Avenue, Suite 10
Mililani, HI 96789

January 1992

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U.S. Army Corps of Engineers
Topographic Engineering Center
Fort Belvoir, Virginia 22060-5546

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The overall objectives for Phase I were to develop the conceptual design for a Hyperspectral Gas Analysis System (HyGAS) for gas detection and identification and to show the feasibility and applicability of this system for real time, spectrum data-base-referenced, processing of high spectral resolution image data, and "hyperspectral" data of gases in a tactical environment. It is concluded that a Hyperspectral Gas Analysis System (HyGAS) can be designed and built which would provide for real time identification and analysis of gas spectra from hyperspectral and ultraspectral imaging sensors.

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HYPERSPECTRAL GAS ANALYSIS SYSTEM (HyGAS™) PHASE I FINAL REPORT

SUMMARY

The overall objectives for Phase I were to develop the conceptual design for a Hyperspectral Gas Analysis System (HyGAS™) for gas detection and identification and to show the the feasibility and applicability of this system for real time, spectrum data-base-referenced, processing of high spectral resolution image data, "hyperspectral" data, of gases in a tactical environment.

To meet this overall objective the project was broken into five major areas of research:

- Identify key applications for the proposed HyGAS™.
- Develop a conceptual design for HyGAS™.
- Define the ultraspectral subsystems.
- Produce a design for probabilistic throughput.
- Produce a design for the merged hyper- and ultraspectral gas data bases.

All of the main objectives of Phase I were accomplished and the following conclusions were drawn:

- The technical and scientific requirements for processing of gas spectra are historical and well defined.
- The Hyperspectral Image Processing System (HIPS™) can be easily adapted to use for analysis of hyperspectral and ultraspectral gas spectral data. Fourier transform and interferogram analysis algorithms are easily added to the HIPS™ library of processing functions.
- HIPS™ presently incorporates spectral search of a data set (image cube) against a spectrum library. Spectral matching routines retrieve candidates from the list of available spectra with probability constraints on the selections.
- Several parallel processing and multiprocessor systems are available for integration with HIPS™ which provide rapid, realtime processing of spectral and spatial data for gases.
- Spectrum libraries are available and can be accommodated by modification of the HIPS™ Spectral Search Library.

It is concluded that a Hyperspectral Gas Analysis System (HyGAS™) can be designed and built which would provide for real time identification and analysis of gas spectra from hyperspectral and ultraspectral imaging sensors.

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I. Technical Objectives of Phase I

The overall objectives for Phase I were to develop the conceptual design for a Hyperspectral Gas Analysis System (HyGAS™) for gas detection and identification and to show the the feasibility and applicability of this system for real time, spectrum data-base-referenced, processing of high spectral resolution image data, "hyperspectral" data, of gases in a tactical environment.

To meet the overall objectives the project was broken into five major areas of research:

1. Identify key applications for the proposed HyGAS™.

   Identify several key applications for the proposed Hyperspectral Gas Analysis System (HyGAS™) and determine the functionality and operational requirements of a HyGAS™ for each of these applications.

2. Develop a conceptual design for HyGAS™.

   Develop a conceptual design for an integrated HyGAS™, including the data base and analysis components to be implemented in a parallel processing environment if practicable. This shall include the definition of requirements for the top-level driver to the system, a design for the procedure-based processing (PBP) framework for the top-level system, and a design for the "point-and-click" user interface.

3. Define the ultraspectral subsystems.

   Define the ultraspectral subsystems, including the the required input parameters and constraints. Identify existing software for performing gas spectrometry that may be modified and integrated into HyGAS™.

4. Produce a design for probabilistic throughput.

   Produce a detailed design for the throughput of probabilistic information that is generated by appropriate components of the system.

5. Produce a design for the merged hyperspectral and ultraspectral gas data base.

   Design an integrated data base system for hyperspectral and ultraspectral gas analysis which includes the identification of requirements, sources, and methods for populating the data base.

II. Research Conducted in Phase I

The following eight tasks were defined under which the technical objectives would be accomplished:

- Conduct requirements survey.
- Conduct software and remote instrument survey for gas spectrometry.
- Design overall system.
- Design gas spectrum data base format.
- Design user interface structure.
- Conduct survey of existing data bases.
- Design parallel processing interface if practicable.
- Design integration of processing system and gas spectrum data base.

Each of these tasks is described in more detail in separate subsections. The results of the research accomplished by each of these tasks are reported in Section III. These results are formulated into a comprehensive description of the Hyperspectral Gas Analysis System that will be implemented under HyGAS™ Phase II.

II.1 Conduct Requirements Survey

This task involved the following activities to determine requirements for gas detection, identification, and analysis for tactical and strategic, commercial, scientific, and environmental applications:

- contacting potential users,
- reviewing existing requirements surveys,
- following up on groups contacted by the HyGAS™ COTR, and
- determining whether ultraspectral analysis is a requirement and in which cases hyperspectral analysis would suffice.

II.2 Conduct Software and Remote Instrument Survey for Gas Spectrometry

This task involved contacting organizations which produce and or use software and instruments for gas detection, identification, and analysis to determine availability of

- spectral/image processing software,
- gas detection instruments, nonimaging and imaging, and
- requirements for gas detection instruments.

II.3 Design Overall System.

This task involved the following:

- design of the HyGAS™ machine platform and basic software configuration,
- determination of the elements of HIPS™ which are applicable to gas analysis, and
- determination of the components which need to be added to HIPS™ to meet ultraspectral requirements.

II.4 Design Data Base Format.

This task involved the following:

- determination of parameters pertinent to spectrometric gas detection and identification,
- determination of the availability and applicability of laboratory and field data relative to gas detection, identification and analysis requirements, and
- design of software for the construction of a gas data base, based on a "learning" environment in which the user may include new information.

II.5 Design User Interface Structure.

This task involved the following:

- design of a procedure-based processing (PBP) interface around a gas analysis scenario.

II.6 Conduct Survey of Existing data bases.

This task involved the following activities to determine the availability, nature and cost of gas spectra data bases:

- contacting gas detection instrument companies and laboratories,
- following up on contacts made by the COTR, and
- contacting additional groups which are accomplishing gas detection and analysis.

II.7 Design Parallel Processing Interface.

This task involved the following:

- determination of the applicability of parallel processor and multiprocessor technology to the gas analysis problem,
- development of a design for a high-level parallel processor or multiprocessor system to link to HIPS™ if practicable, and
- development of a detailed design for the throughput of probabilistic information for gas detection, identification and analysis.

II.8 Design Integration of Processing System and Gas Spectrum Data Base.

This task involved the following:

- designing a HIPS™-compatible interface between the parallel processor or multiprocessor identified in Section III.7 and the gas spectrum data base format mentioned in Section III.4.

III. Results of Phase I

This section summarizes the results of and conclusions from the research conducted in Phase I. The results are presented in the form of a complete conceptual design of the system to be implemented in Phase II, including descriptions of the software system itself and its capabilities.

III.1 Introduction

One of the major areas of research during Phase 1 was a detailed evaluation of the current state of the technology for remote detection and identification of gases. Twenty-two contacts (see Table 1)with various government organizations and agencies, industries, and academic institutions are broken down into the following groups:

- 4 government
- 17 industry
- 1 academic

Contacts are categorized further as:

- 10 providing requirements, scientific and technical, for gaseous data analysis;
- 9 providing spectrum and image processing software;
- 11 providing gas detection instruments and designs, point and imaging;
- 3 providing parallel processing applications;
- 12 providing gas spectrum libraries; and
- 27 references to technical papers on requirements, applications and techniques for gas detection and identification.

Table 1: Contacts

Aldrich Chemical Co. 940 W. St. Paul Ave. Milwaukee, WI 53233-2681 mailing address: P.O. Box 355 Milwaukee, WI 53201-0000	IR libraries.	(414) 273-3850 FAX (414) 273-4979 1-800-231-8327
BOMEM, Inc. 4 New Casho Mill Road Newark, Delaware 19711	Gas sensors; Analysis systems.	Jim Malone (302) 366-8260
David Sarnoff Research Center	Parallel processing; Princeton engine.	David Weir (609)734-2028
E-Systems	N-cubed processor; Parallel processing.	Bob Johnson (214)205-7613
EG&G 2621 Loses Road Las Vegas, NV 89125	Instrument (CASI); Data; Software needs.	Lee Balick (702) 295-0029
EG&G Mound Applied Technologies P.O. Box 3000 Miamisburg, OH 45343-3000	Hazardous gas detection.	Rene Smith, buyer (513) 865-3490
Grumman Aerospace, Huntington Long Island, NY	Gas modeling; HCL&methane gas libraries; Smoke stack plume studies; Mobile nonimaging sensors.	Dr. Jerry Krassner (703) 875-8400 (Rosslyn, VA)
Infrared Analysis, Inc. 1424 North Central Park Ave. Anaheim, CA 92802	IR reference libraries and calibrations.	Dr. Phil Hanst (prev. with EPA 30 yrs) Steve Hanst (son) (714) 535-7667
Johnston Atoll	Air monitoring.	Nollie Swynnerton Southwest Research Inst. (808) 621-3044 exts. 3364 or 3369
Lockheed Missiles & Space Co., Inc. P.O. Box 3504 Sunnyvale, CA 94088-3504		Bill Lynch (408) 742-3132
Mattson Instruments, Inc. 1001 Fourier Drive Madison, WI 53717	Instruments; Software; Variety of IR libraries.	(608) 831-5515 FAX (608) 831-2093
MTL Systems, Inc. 3481 Dayton-Xenia Rd. Dayton, O 45431-0299	Instruments	Dave Kelch (513) 426-3111
Naval Surface Warfare Center Dahlgren, VA (HyGAS™ COTR Contact Only)		Protection System Department; Magnetic, Chemical, and Biological Warfare Counter- measures Division; Chemical Warfare Shipboard Systems Branch
Nicolet Instrument Corp.	Instruments; Software;	(608) 273-5004

5225 Verona Road Madison, WI 53711-4495	FTIR libraries; Vapor phase library.	
Photometrics Ltd. 3440 East Britannia Dr. Tucson, Arizona 85775-0615	CCD spectroscopic detection systems.	(602) 889-9933 FAX (602) 573-1944
Research Systems, Inc. 777 29th St., Ste. 302 Boulder, CO 80303	IDL software.	(303)786-9900 FAX (303)786-9909
Sadtler 3316 Spring Garden Philadelphia, PA 19104	IR libraries.	Tom LeVeque (215) 382-7800
SETS Technology, Inc. 300 Kahelu Ave. Ste. 10 Mililani, HI 96789	Instruments, software	(808)625-5262
SpecTerra Systems Pty. Ltd. Dalkeith, Western Australia	Instrument for passive detection.	Dr. Frank Honey 61-9-389-8050
U.S. Army Chemical Research and Development Center (CRDEC) Aberdeen Proving Ground, MD 21010-5423	Remote sensing R&D for gas detection and analysis	Chemical Division Research Directorate - Organic Chemistry Branch; Analytical Research Directorate - Spectral Analysis and Standoff Detection Branch; Attn:SMCCR-RRSL Dr. Bob Kroutil Kirk Phelps (301) 671-5527
U.S. Army Nuclear and Chemical Agency Fort Belvoir, VA (HyGAS™ COTR Contact Only)		
University of Denver Dept. of Chemistry Denver, Colorado 80208	Pollution monitor; UV libraries.	Dr. Donald Stedman (303) 871-2580 FAX: (303) 871-2587

III.2 Requirements survey

Step 1 of the Phase 1 study was to conduct a requirements survey which focused on four areas of applications of gas detection, identification, and analysis:

- Tactical and strategic
- Commercial
- Scientific
- Environmental

Table 1 lists the organizations contacted. Of 22 contacts made with various government installations and agencies, industries, and academic institutions, 10 provided requirements information.

We found that the technical and scientific requirements for spectral processing of gas spectra are historical, and systems for the acquisition, detection, and analysis of gases have been in use for many decades. Refinements to these are continuous, keeping pace with new instruments for acquisition of gas data and innovations in data analysis. New analysis techniques include

- Fourier transform infrared spectroscopy,
- interferogram analysis, and
- imaging spectroscopy (which adds the spatial dimension to gas analysis).

Two requirements documents for material identification were reviewed which yielded many gas detection and analysis requirements. These will be reported to the HyGAS™ COTR independent of this report.

One of the most significant contacts was a follow-up on a contact made by the COTR, Mr. Sam Barr, with Dr. Bob Kroutil, U.S. Army, CRDEC, Aberdeen Proving Ground, Md. SETS Technology senior scientist Dr. Tom Lundeen and Mr. Bob Chatman visited Dr. Kroutil on two separate occasions and telephoned Mr. Steve Gotoff, also at Aberdeen. SETS and Aberdeen scientists exchanged views on gas detection methodology, point and imaging; discussed advantages and disadvantages of interferogram and spectrum matching approaches to detection and identification; arranged for the transfer of digital gas spectra from Aberdeen to SETS (not yet accomplished as of this report); and discussed the possibility of SETS receiving Aberdeen spectrum processing algorithms for use in the HyGAS™ system. Details from the interaction with Aberdeen are interspersed throughout this report and are noted as such.

The results of the requirements survey are broken down into five areas:

- gas detection phenomenology,
- tactical and strategic,
- commercial,
- scientific, and
- environmental applications.

For each of the areas the organizations contacted will be referenced and requirements summarized, focusing on the applications, phenomenology observed, types of instruments used, and data processing methods which concerned and in some cases constrained the efforts of the organizations contacted.

III.1.1 Phenomenology

Successful gas detection, identification, and analysis of spectra and spatial occurrence (concentration and rate of dispersion; distribution, both horizontal and vertical) for a gas are a function of understanding gas phenomenology, i.e., the way gas reacts to and with its environment, chemically and physically.

III.1.1.1 Temperature and Concentration

Gas, like the atmosphere, is a medium made up of relatively large molecules, which absorb, transmit, and emit energy, the magnitudes of which are based upon the temperature, concentration, and constituency (species). The occurrence of absorption, transmission, or emission depends upon one of three thermodynamic conditions. In the first, an intervening gas absorbs radiance when its temperature is less than that of its background. In the second, a gas transmits radiance when its temperature is equal to that of the background. In the third, a gas emits radiance when its temperature is greater than that of the background. Thus, the only thermal conditions which allow a gas to be detected are when it is of lesser or greater temperature than its background.

Field tests of gas phenomenology conducted by Dr. Kroutil have shown that almost immediately after dispersion, the temperature of a gas will be found to be at least 1.5 to 3°C different than that of the ambient atmosphere and can be as different as 30°C. Existing gas detection systems have a sensitivity of 0.10°C, thus, as a function of temperature difference, gases are almost always detectable. A curious phenomenon reported by Dr. Kroutil indicates that a dispersing gas can fluctuate between absorption and emission conditions at a rate of once every 3–5 seconds, a phenomenon which is also spatially variant.

A gas can absorb energy from any substance which is reflecting or emitting, provided the energy is sufficient to activate the electronic, vibrational, or rotational states of the molecules. Sources of energy can be chemical, such as the reactions with other gases in the atmosphere, CW weapon discharges, or in gas plumes; or physical, such as emission from the atmosphere or a physical surface (the Earth), or from emitted and reflected solar irradiance.

Detectability is a function, not only of the temperature, but also, of the concentration of the gas, the band strength, and the path length through the gas cloud. The strength (i.e., amplitude) of the absorption or emission feature in the gas spectrum is related to ΔT and proportional to the product of the concentration, the path length, and the band strength (Beer's Law). Thus, for a gas to be detectable it must differ in temperature from the background and must be of sufficient concentration with respect to the spectral resolution and signal-to-noise ratio (SNR) of the acquisition system to be differentiated from noise.

III.1.1.2 Waveband Regions of Gas Absorption and Emission Bands

The occurrence of gas absorption and emission bands is of primary importance to detection and analysis. Most gases of interest to this study tend to be made up of large molecules. As a result of this and the fact that gases are independent molecules (not attached to others as is the case for the solid state) absorption and emission result primarily from vibration and rotation of the molecules, and produce spectral lines or narrow bands. The waveband region of interest for gas analysis for optical sensors (refractive, 0.2 to 20 μm) tends toward the mid- (2.5 to 8.0 μm) to far infrared (8.0 to 20 μm); indeed, the region of 8.0 to 14.0 μm is customarily referred to as the "fingerprint region" for gas identification. It is thought that the overtones of the vibration and rotation in these regions are too weak to be detected by sensors operating from 0.3 to 2.5 μm.

However, one should not minimize the occurrence of electronic transitions and vibrational modes in the ultraviolet, visible, and near-infrared region for some gas species, e.g., ozone, in the ultraviolet.

III.1.1.3 Spectral Features of Gases

Spectral features of gases include absorption and emission lines. These features are used to detect gases, differentiate them one from another, analyze the quantum mechanical effects of gases interacting with energy such as emission and absorption, and are necessary for the analysis of the species, temperature and concentration of the gas. These lines are very narrow, ~$\Delta\lambda/\lambda$ of 0.001, and are detectable in the field only with what we are calling "ultraspectral sensors." Atmospheric models such as FASCODE are used to model atmospheric and gas absorption and emission lines. For all but the smallest and most simple molecules, the fine line structure of gases is blended together, and is subdued or erased.

When taken in the aggregate, this line structure is sometimes sufficient to define bands which have the following differentiating features: location, the position of the band center; band strength, width-at-half-height; amplitude, base to full height; and slope of the sides of the distribution curve defining the band. These features are used to detect and differentiate gases, one from another. They are broad enough, ~ $\Delta\lambda/\lambda$ of 0.01, to be detected using "hyperspectral" sensors, however, they are rarely detected using multispectral sensors, $\Delta\lambda/\lambda$ of 0.1 or greater. These features, occur as inputs parameters for gas and atmospheric band models such as LOWTRAN and are used in spectral matching algorithms.

Dr. Kroutil reports that an absorption or emission band width of 16 wavenumbers, which in the gas fingerprint region of 10 μm yields a $\Delta\lambda/\lambda$ of 0.016, is consistent with the spectral discrimination capability of hyperspectral sensors (Dr. Kroutil is, however, presently using a single field of view, nonimaging sensor which has a resolution of 8 wavenumbers.).

Spectral analysis and matching techniques use various combinations of spectral features. It is important to note that the absorption and emission spectra for a gas are not identical (do not superimpose), rather, they are mirrored and the <u>emission spectrum</u> is shifted toward the longer wavelength (lesser energy). <u>This means that a data base of gas spectral features must contain a set for emission and a set for absorption with the appropriate adjustment in line and band center positions</u>. The impact of this shift on hyperspectral and ultra spectral data analysis should be investigated in Phase II.

III.1.1.4 Detection and Identification Methodologies

Dr. Kroutil reports two general methods for gas detection and identification: spectrum matching and interferogram processing. The spectral matching technique is typically used with staring sensors in which case the background is not changing. The interferogram technique is typically used when the background is changing rapidly as in airborne imaging. In either case, the sensor (spectrometer) is aimed in the direction of an expected gas event. The initial samples recorded and analyzed are, ideally, those of the background (atmosphere or terrain). At the occurrence of the gas event, the combined background and gas spectrum are recorded. Spectrum matching requires the subtraction of the gas spectrum from that of the background, thus, data taken over time are differenced and a "non-zero" value trips the "alarm." The requirement for a non-changing background, for successful spectrum matching, is evident. Subsequently, the gas spectrum, the difference spectrum, may be matched against a library of candidate spectra to identify the gas. In the case of interferogram analysis the interferogram of the scene is recorded and processed to separate the background portion (central peak) from the gas portion (the outer portion or "wings") of the interferogram and to extract signal parameters characteristic of a specific gas. The separation of the portions of the interferogram containing the background and gas information negates the requirement for a non-changing background, as was required for spectrum matching. The resultant parameters are compared with a library of candidates and a match generates an alarm. Both the spectrum matching and the interferogram methods can be used by tactical self-contained, automated units or by an analyst at at a workstation. Sources for the gas detection can be either nonimaging or imaging sensors.

The interferograms are produced by Fourier Transform Infrared Spectrometers (FTIR). The center burst of the interferogram represents the broad band spectral components typical of the background materials, solids or liquids. The wings of the interferograms contain the narrow band or line components, presumably of the gas in question. As one progresses outward from the center burst the signal-to-noise ratio falls off. The interferogram must be processed, prior to analysis, to reduce the effects of the noise. Typically, a "short segment" on the wing of the interferogram is analyzed for evidence of gas spectra, by means of one of several pattern recognition techniques, e.g., multiple discriminant analysis. These parameters, typically the amplitude and frequency of the signal, are matched against a data base of parameters for candidate gases. This process of analyzing only the short segment eliminates the need for background subtraction, by avoiding the center burst, the background.

Presently, gas spectra cannot be extracted from the short segments of the interferogram using Fourier transformation; there are too few points to be analyzed. However, investigations are underway in the use of maximum entropy transformations (see papers by Kroutil referenced in this report). This technique is one of a class of "super-resolution" techniques and is more difficult computationally than the Fourier transformation. It is however a superior technique in that it eliminates the need for background subtraction because it is derived from the interferogram. This technique may hold promise, but needs further development.

A HyGAS™ system could support any of these algorithms with matching against a search library populated with gas spectra or parameters.

III.1.1.5 Detection Systems

Detection systems are of two types: nonimaging and imaging. Discussions with the organizations we contacted indicate the following specifications for gas detection and analysis:

	Hyperspectral	Ultraspectral
Resolution ($\Delta\lambda/\lambda$)	0.01	0.001
NESR	0.01 $Wm^{-2}sr^{-1}$	0.01 $Wm^{-2}sr^{-1}$
NEΔT	0.1 K	0.1 K
SNR at 0.05 albedo	300:1	300:1

NESR, the noise equivalent spectral radiance, is the radiance, r, that yields a signal equal to the system noise. The relationship between SNR and NESR is generally expressed as:

$$SNR_{Rad} = (NESR)^{-1} = \partial(S/N)/\partial r \qquad \text{Eq. 1}$$

NESR is often refered to as the radiance difference that yields a SNR of one. Thus, for an NESR of 0.01 $Wm^{-2}sr^{-1}$, the radiance difference which yields a SNR of one is 0.01 $Wm^{-2}sr^{-1}$. A radiance difference greater than the NESR is able to be discriminated from the system noise.

NEΔT, the noise equivalent temperature difference, is the difference in radiance, converted to temperature, T, that yields a SNR of one. The relationship between SNR and NEΔT is the same as Equation 1, with NEΔT replacing NESR in the second term (Wolfe and Zissis, pg. 19-12). For an NEΔT of 0.1 K, the temperature difference which yields a SNR of one is 0.1 Kelvin (0.1°C). A temperature difference greater than the NEΔT is able to be discriminated from the system noise.

The NESR and the NEΔT are significant when judging the ability of a sensor to discriminate very small differences in and very low levels of reflectance and emittance, and of their derived attributes, such as, spectral contrast, concentration, temperature, and sub pixel presence of materials within a scene.

A sensor which has a spectral resolution, $\Delta\lambda/\lambda$ (λ is wavelength), of 0.01 (typically, a hundred or more wavebands), a noise equivalent spectral radiance (NESR) of 0.01, noise equivalent temperature difference (NEΔT) of 0.1 K, and a signal to noise ratio (SNR) of 300:1 at a 0.05 albedo, is considered to be sufficient for gas detection and identification: a hyperspectral system. However, the precise, quantitative, determination of concentration (to better than a factor of 2) and temperature (linked to the determination of concentration) requires an ultraspectral system. This system is generally defined by the same criteria as the hyperspectral system, but with an increase in spectral resolution, $\Delta\lambda/\lambda$, 0.01 to 0.001 (typically, a thousand or more wavebands). One problem with increasing the spectral resolution is that the SNR decreases (under equivalent sampling condition, e.g., sampling time). Consequently, the gas detection problem is optimized by balancing spectral resolution against band separability for the gases and waveband region of interest.

For real time warning systems the sampling and data analysis rate must be on the order of 5 to 10 per second; the output can be analyzed by a user, interactively, at a remote workstation. For non-real time systems the sampling rate can be lower and the analysis can include scientific analysis, again, at a user interactive workstation. Laboratory spectrometers fit the specifications for an ultraspectral system, because, unlike their field or airborne counterparts, no tradeoffs have to be made with resolution to obtain the necessary integration time, data transfer, or field of view.

III.1.1.6 Spatial Phenomena of Gas Events

Spatial phenomena of gas events include:

- location(s) of primary event(s) or origin(s) of dispersion(s);
- concentration and contouring;
- dispersion rate and direction;
- precipitation and adsorption on, and absorption by background surfaces, e.g., contaminated soil and water;
- effects of gas and byproducts or altered products on the local environment, e.g., vegetation stress (very evident when viewed in the appropriate waveband); and
- topographic influences on the gas event, such as wind shadows and traps (canyons, forested areas), thermal shadows, thermal sinks and emitters (cover types such as large bodies of rock, unvegetated areas sand and soil), and dispersion corridors (topographic valleys and barriers).

Addressing these phenomena requires a full complement of spectral and spatial analysis tools, many of which are common to image and spectral processing systems such as HIPS™.

Spatial analysis could be integrated with the spectral analysis by the following steps:

- spectral image acquisition,
- processing to detect and identify (hyperspectral) and calculate concentration and temperature (ultraspectral),
- calculation of the <u>rough order abundance</u> (factor of 2) of gas species by estimating gas temperature or by fitting the Planck Function (hyperspectral), or calculation of the <u>precise concentration</u> of gas species using absorption/-emission line strength (ultraspectral) for each pixel,
- calculation of contour maps showing gas concentration and temperature gradients,
- determination of the center of dispersion of the gas,
- differencing of temporal images to calculate the rate, direction, and spatial extent of gas movement and dispersion, and
- correlation of the spatial phenomenon with tactical, feature, and topographic map (or digital terrain) data and with the physical phenomenon of the surface materials (temperature, type, etc.) by porting data to a geographic information system (GIS) for information extraction and decision making.

This scenario would require adding spatial processing algorithms to HIPS™ for HyGAS™ to provide:

- Contour maps of temperature profiles.
- Contour maps of gas clouds (including, plume topography) based on spectral abundance.
- Gas cloud migration patterns based upon time-dependent measurements.
- Maps based upon the likelihood that a particular gas is present.

It is important to note that this scenario is easily adapted to downlooking, uplooking, and sidelooking image acquisitions. This scenario can also be run using gas modeling algorithms and data as a training and planning tool for tactical/strategic decision makers and civil investigators alike.

III.1.2 Tactical and Strategic Requirements

The tactical and strategic requirements were basically differentiated by observational context. The tactical context was typically defined as time dependent, short duration gas events such as those associated with the battlefield or potential battlefield, and the strategic context as persistent, long duration, or predictable gas events such as are associated with production facilities.

III.1.2.1 Tactical Requirements

Tactical requirements are primarily focused on the detection and identification of chemical warfare (CW) agents for alarming purposes and are driven by the need for real-time, rapid reporting. The requirement which motivated the HyGAS™ study is for a gas detection capability coupled with spatial context, i.e, an imaging spectrometer. Current tactical detection instruments are nonimaging spectrometers which use one of several sampling techniques:

- sampling a field of view defined by a single detector element,
- sampling a range (an arc) defined by many separate detector elements of fixed field of view sampling contiguously over an arc, and
- sampling over a continuous path from an airborne platform using the two configurations previously listed.

The data acquisition and analysis for the current, nonimaging sensors includes rapid acquisition rates varying from 5 to 50 samples per second. The data is acquired as spectra and/or interferograms and is processed onboard the sensor system. Spectral data is analyzed using signals processing algorithms and spectral matching against a library of candidate CW agents. The spectral matching technique involves the subtraction of the gas spectrum from that of the background and is dependent upon a precise knowledge of the background spectra. Consequently, his technique is limited to use with data recorded by stationary sensors for which the background materials, hence, the spectra do not change. The interferogram technique, on the other hand, enables acquisition of data in situations in which the background against which the gas event occurs is rapidly changing, e.g., airborne acquisitions over terrain of varying cover. Interferogram data which contains both the background information and the gas information is processed using pattern recognition techniques. The results are matched to a list of parameters characteristic of candidate CW agents. While gases can be detected and identified using this technique, it is not possible to extract spectra from the interferogram: spectra may be acquired by the same instrument as that which provides the interferogram (a Fourier transform infrared (FTIR) spectrometer), but must be analyzed independently. An example of an instrument using both the spectrum matching and the interferogram processing techniques is the XM-21, Remote Sensing Alarm, presently undergoing development and field (ground and inflight) testing by Dr. Kroutil.

Additionally, there are tactical requirements for the analysis of the alteration products, as well as gases, created when certain CW agents which have a high freezing point settle onto the battlefield, e.g., mustard gas. A hyperspectral sensor would be appropriate for the detection of the "solid state" as as well as the "gaseous state" of these agents. The image would provide the required spatial context and the data could be easily integrated with map data in a geographic information system for planning purposes.

III.1.2.2 Strategic Requirements

Strategic requirements are primarily focused on the detection and identification of gaseous precursors to the production of various chemicals, of gaseous effluents indicative of specific industrial processes and events and of exhaust plumes of various vehicles. Detection instruments are ground based and airborne, nonimaging (typically point systems) and imaging spectrometers, either hyperspectral or ultraspectral. The sampling techniques for the point system would be similar to those stated in the tactical requirements section with the exception of a lower sampling rate required.

The data is acquired as spectra, interferograms, or spectral imagery and is typically processed using an accompanying field deployable work station or in the case of airborne sensors, processed using a processing system onboard the aircraft or at a ground facility. Spectral data would be analyzed using signals or interferogram processing algorithms and matching against a library of candidate gases. The COTR for HyGAS™, Mr. Sam Barr, has provided a list of precursor gases and sample spectra from two separate agencies concerned with strategic requirements.

Strategic requirements also address the effects of gases on local and geographically extended environments. Like their tactical counterparts, these would be addressed most appropriately by an imaging spectrometer (hyperspectral sensor). The image would provide the required spatial context for the occurrence. The image data could be easily integrated with map data in a geographic information system for planning purposes.

III.1.3 Commercial Requirements

Commercial requirements focus primarily on the monitoring of industrial processes. Monitoring devices are typically mounted on or in the vicinity of effluent discharge ports such as smokestacks and exhaust ducts. These monitors are typically nonimaging, point spectrometers. Data sampling and processing rates would be set as necessary for the specific application and processing could be automatic for alarming or continuous monitoring devices, or analyst interactive for engineering studies. Obvious applications for imaging spectrometers would be for aircraft or rocket engine exhaust plume monitoring in which the species, distribution, temperature profile, rates of dispersion, and persistence of gases have spatial significance. Dr. Jerry Krassner, Grumman Aerospace, provided requirements for monitoring aircraft and rocket engine exhaust for CO, HCl and water vapor content. Grumman has an extensive array of field spectrometers (nonimaging) and makes use of gas modeling algorithms. The sensors used for these commercial applications would typically be considered ultraspectral sensors (high spectral resolution).

There are many other imaging spectrometers used by astronomical researchers for stellar and planetary atmospheric gas studies. The resolution of these spectrometers is typically $\Delta\lambda/\lambda$ of 0.001 to 0.0001. These spectrometers are special purpose and not suitable for field or airborne deployment at this point in time.

III.1.4 Scientific Requirements

Scientific requirements are typically focused on extended analysis in which data acquired using high resolution spectrometers, point and imaging, is analyzed in great detail in a highly user-interactive environment. The primary example is the spectral analysis of the atmosphere of the Earth, planets, the Sun, and stars. Absorption and emission line data provide information on composition, temperature, spatial distribution (horizontal and vertical), dispersion rates, rate of movement, etc. An example is the study of the concentration of the ozone in the atmosphere and its spatial occurrence. This is accomplished using the spectrometers operating in the ultraviolet and far infrared regions of the spectrum where ozone absorption is prominent. An example of an imaging spectrometer for scientific applications is the Visible and Infrared Imaging Spectrometer (VIRIS™, SETS Technology, Inc.) which was designed for use at the Mauna Kea Observatory, Hawaii. Data processing is typically accomplished with user-generated algorithms on highly interactive work stations; the spatial and temporal processing is essential to provide context to the spectral data.

III.1.5 Environmental Requirements

Environmental requirements for gas detection and analysis are listed last because they are similar if not identical to the tactical and strategic, commercial, and scientific. As with the tactical, discharge from nuclear reactors. As with the strategic and commercial requirements, they are focused on monitoring gas discharge from industrial processes and toxic waste storage and disposal sites; the content, persistence, dispersion rates and direction of movement of smokestack effluents, oil well fire plumes, etc.; atmospheric pollution/air quality and their spatial distribution; and the effects on the local and extended environment, such as vegetation stress. Resolution requirements vary from $\Delta\lambda/\lambda$ of 0.05 (hyperspectral) to $\Delta\lambda/\lambda$ of 0.002 (ultraspectral). Waveband regions of interest vary from the near to far infrared, with the 3–5μm and 8–12μm regions of particular importance, especially the hydrocarbon stretch in the 3–5μm region.

An example of an environmental requirement was given by Mr. Mark Maguire (replaced by Mr. Nollie Swynnerton), Chief Lab Technician for Southwest Research Institute, the subcontractor responsible for monitoring incineration emissions on Johnson Atoll (see Table 1). Gas monitoring is performed by the Automatic Continuous Air Monitoring System, a near-real-time monitor that uses a gas chromatograph, produced by ABB Process Analytics in Lewisburg, W. Virginia.

Another example of environmental applications is in the study of "greenhouse" gases, nutrient changes caused by wildfires, and the effects of aerosol pollutants in the atmosphere on global warming. These studies are being conducted by NASA/Ames Research Center using the "Wildfire" imaging sensor made by Daedalus. The Wildfire consists of a 50-channel spectrometer with 10 bands in the 8.2 to 12.7 μm region, and 40 bands in the 1.15 to 5.40 Mm region; $\Delta\lambda/\lambda$ is on the order of 0.05, in the range of hyperspectral sensing. Daedalus is developing a new hyperspectral sensor, the Multispectral Infrared/Visible Imaging Spectrometer (MIVIS) which consists of 10 channels in the 8.2 to 12.7 μm region, 64 in the 2 to 2.5 μm region, 8 in the near infrared, and 20 in the visible region.

III.2 Conduct Software & Remote Instrument Survey for Gas Spectrometry

Of the organizations contacted by the HyGAS™ contractor nine provided information on spectrum and image processing software (see Table 2), and 11 provided information on gas detection instruments and designs, point and imaging (see Table 3). Detailed information on many of these products is archived at the HyGAS™ contractor facility and is available for review.

Table 2: Software

BOMEM, Inc.	Spectral analysis package.
Grumman Aerospace	Gas modeling software for line and band spectra.
Infrared Analysis, Inc.	I-GRAMS (Infrared Gas Research And Measurement System).
Mattson Instruments, Inc.	FIRST (Fourier Infra-Red Software Tools).
Nicolet	QUANT (QUANTitative analysis software).
Photometrics Ltd.	RDS200 - CCD Spectroscopic Detection System with SpectraCalc - advanced spectroscopy software.
Research Systems, Inc. (RSI)	IDL software package - (Spectral Image Processing System).
Sadtler	Spectral search software and spectrum libraries.
SETS Technology, Inc.	HIPS™ (Hyperspectral Image Processing System).

Table 3: Instruments

Company	Instrument	Type	Range overall	Resolution typical
ABB Process Analytics	"Automatic Continuous Air Monitoring System"	Field		
BOMEM, Inc	FTIR Spectrometer - DA2 Series	Field, Point	400-50000 cm-1	to 0.013 cm-1
	FTIR Spectral Radiometer- MB Series	Field, Point	0.75-20 µm	selectable 1-128 cm-1
	FTIR Spectrometers	Laboratory, Point		
Daedalus	"Wildfire" IR Imaging Spectrometer	Airborne, Imaging	1.15-12.7 µm	0.05 Δλ/λ
	Multispectral Infrared/Visible Imaging Spectrometer - MIVIS (under development)	Airborne, Imaging	0.4-12.7 µm	0.02–0.05 Δλ/λ
Infrared Analysis, Inc.	MIDAC Interferometer (used by US Army CRDEC, Aberdeen)	Field, Point	800– 1200 cm-14 cm-1	
ITRES Instruments, Inc.	CASI	Airborne, Imaging	.430-.870 µm	0.005 Δλ/λ
Mattson Instruments, Inc	FTIR Spectrometers	Laboratory, Point	750-4000 cm-1	to 0.06 cm-1
MTL Systems, Inc.	Airborne Spectroradiometric Imaging System (ASIS)	Airborne, Instrument	0.4–2.5 µm	
			0.4–1 µm	0.04 Δλ/λ
			1.1–1.8 µm	0.09 Δλ/λ
			2.00 – 2.5 µm	0.007 Δλ/λ
	Airborne Thermal Imaging System (ATIS)	Airborne, Instrument	0.4–12.0 µm	
			0.4–1 µm	broadband
			3-5 µm	broadband
			8-12 µm	broadband
			8-12 µm	0.1 Δλ/λ
			8-12 µm	0.05 Δλ/λ
Nicolet Analytical Instruments	FTIR Spectrometers - Sys 740	Laboratory, Point	50-15000 cm-1	selectable to 0.3 cm-1
SETS Technology, Inc.	Visible and Infrared Imaging Spectrometer - VIRIS™	Field, Imaging	1.0-2.5 µm	0.01 Δλ/λ
	Visible and Infrared Imaging Spectrometer - VIRIS™ (spectrometer to 2.5 µm, detector array to 5.0 µm) (under development) (design)	Field, Imaging	0.35-5.0 µm	0.01 Δλ/λ
	Variable Spatial Resolution Infrared Spectrometer - VSRIRS™ (design)	Field, Imaging	1.0-12.0µm	0.001 Δλ/λ
SpecTerra Systems Pty. Ltd.	Interferometer	Field, Imaging		
Other systems, astronomical	Various special purpose imaging spectrometers	Field, Imaging		0.001–0.0001 Δλ/λ

This survey showed that the technical and scientific requirements for the processing and analysis of gas spectra are historical and systems for the acquisition, detection, and analysis of gases have been in use for many decades. Refinements to these are continuous and include Fourier transform infrared spectroscopy, the use of interferogram techniques, and the application of imaging spectrometers to acquire gas spectra, adding the spatial dimension.

Spectral processing software has been in use for many decades and spatial processing software for several decades. Spectral matching and Fourier transform analysis are common categories with the recent addition of interferogram processing. The former two are widely available, however, sometimes in specialized form and for use with specialized spectral processing equipment. There is no processing system known to us which incorporates both of these categories of processing into a consolidated unit.

The HyGAS™ study has shown that the Hyperspectral Image Processing System (HIPS™), developed under an SBIR contract with the U.S. Army, Topographic Engineering Center, Ft. Belvoir, Va., COTR, Sam Barr is in many ways applicable to and easily adapted for the analysis of hyperspectral and ultraspectral gas spectral data. The HIPS™ presently incorporates spectral search of a data set (image) against a spectrum library. Spectral matching routines provide candidates from the list of available spectra with probability constraints on the selections. Fourier transform and interferogram analysis algorithms are available from several sources and are easily added to the HIPS™ library of processing functions.

Many excellent instruments for the detection and identification of gases have been and are in use in laboratory and in the field of which point detection systems are the majority with far fewer imaging spectrometers, especially field deployable (see Table 3). Designs for imaging spectrometers are available which meet the specifications for gas detection, SNR greater than 300:1 at a 0.05 albedo, a NESR of 0.01, a NEΔT of 0.1 K, and $\Delta\lambda/\lambda$ of 0.01. The limiting factor is the insufficient detector technology in fabricating large detector arrays for the mid- and far infrared regions so critical to gas detection.

III.3 Design overall system.

HyGAS™ will consist of three primary components:

- the Computational Algorithms (**Section III.3.7**),
- the Spectral Data Base (**Section III.4 and III.8**), and
- the User Interface (**Section III.5**).

The User Interface links the user with the Computational Algorithms which in turn utilizes the Spectral data base for performing the gas analysis.

III.3.1 Hardware

The initial software design and testing will be preformed on a SUN SPARCstation II. This system will act as a front end to any of the parallel processors tested.

III.3.2 Operating System

The system will be developed to operate under a POSIX (standardized UNIX) operating system to provide maximum portability to other computing platforms. Initial development will take place under Sun's version of UNIX, SunOS, version 4.1 or higher.

III.3.3 Programming Tools

The system will be built and maintained utilizing state-of-the-art programming tools, including a CASE (Computer-Aided Software Engineering) system; an automated software build system; a source code control system, and advanced debugging tools. CASE provides an overall environment for advanced software engineering. Automated build software allow systems to be rebuilt repeatedly and efficiently , avoiding unnecessary compiling, linking of unmodified code, and tracking complex code dependencies. A source code control system allows numerous programmers to work on the system simultaneously without the duplication and/or canceling out of efforts often found in multiple-programmer situations. Debuggers allow programmers to take code apart piece by piece to correct malfunctions.

III.3.4 On-line Help

The system will contain a two-tier help system, the first level giving a short statement of help information, the second giving pages of help, if necessary.

III.3.5 User Documentation

The system will be delivered with a comprehensive User's Manual describing each function, the function's arguments, and how the function works.

III.3.6 Data Handling

The system will be capable of handling data sets data cubes) of any size, limited only by available disk space. The data can be configured to be one, two, three, or four dimensional. The data can be in any of eight data types—byte, unsigned byte, short integer, unsigned short integer, long integer, unsigned long integer, floating point, and double precision. Data from a variety of sources will be handled by routines that will translate the foreign data formats into a native data format.

III.3.7 Capabilities of the Software System

Two categories of software capability are described here. The first category includes general data cube processing functions and the second involves specialized routines used for spectral analysis of gases.

III.3.7.1 General Cube Processing Capabilities

All of the general data cube processing will be handled using HIPS™ which is a generalized hyperspectral data processing system developed by SETS Technology, Inc. under a previous SBIR contract with the U.S. Army, Topographic Engineering Center. This system will be augmented to allow improved handling of ultraspectral data and accomplish additional spatial processing. A highly interactive mode will be added to preform single spectral analysis.

III.3.7.2 Computational Algorithms and Specific Capabilities

It was determined in the Phase I effort that the following specialized data manipulation and analysis algorithms would be needed as a basis of a gas analysis system:

Spectrum recognition and identification algorithms:

- Band encoding of spectral features for comparison with the spectral data base.
- Pattern recognition routines for spectral identification in both the frequency and time domain.
- Spectral search routines for both forward and reverse searches against a library, i.e., data set against library and library against data set..

Data processing algorithms:

- Forward and Reverse Fourier Transforms.
- Convolution routines for decreasing the apparent spectral resolution.
- Deconvolution routines for increasing the apparent spectral resolution.
- Temperature calculations based upon a best fit to a Black Body Curve.

- Calculations of modeled spectrum using the integrated spectral library.

Spatial processing algorithms:

- Contour maps of temperature profiles.
- Contour maps of gas clouds (including plume topography) based on spectral abundance.
- Gas cloud migration patterns based upon time dependent measurements.
- Maps based upon the likelihood that a specific gas is present.

III.4 Design Spectrum Data (Knowledge) Base Format.

Several of the functions in the system will be capable of reading in spectra from a spectral library and using them for comparison or calculation with either the spectra in a cube or with single spectra in the single spectra analysis sub-system.

HyGAS™ will facilitate the addition of data to the gas spectral search library from several sources:

- laboratory and field data,
- data derived from the spectral image (an existing feature of HIPS™), and
- data generated using gas modeling algorithms in HyGAS™.

The first two features are included in HyGAS™ to provide the learning environment in which the user may include new spectral information derived from the scene or from models into existing analysis or scenarios for planning purposes.

The current HIPS™ library system will be augmented to meet the requirements for gas analysis and for use in the thermal infrared. In particular new algorithms will be developed for:

- Band encoding of the data.
  - Band Position
  - Band Strength
- Pattern recognition to support full spectrum matching and interferogram analysis.
- Convolution routines.

III.5 Design User Interface Structure.

HyGAS™ will be designed as an addition to HIPS™, to take full advantage of the work already performed and testing which has been accomplished on that system. However, the new procedures and functions can still be operated independent of HIPS™. Additionally, it is important to recognize that the integration of HyGAS™ hyperspectral and ultraspectral capabilities into HIPS™ preserves the multispectral and hyperspectral functionality of HIPS™ which is essential for the analysis of targets and background features. The following brief description of HIPS is provided as reference.

HIPS is a software package developed specifically for multispectral and hyperspectral image processing and analysis. The philosophy guiding the design of HIPS was to create an easy-to-use exploitation system for manipulating and analyzing the large volume of data—and information—contained in multisensor, multispectral, hyperspectral, and ultraspectral image cube data sets. HIPS, complete with an integrated Spectral Search Library, is used for target discrimination and identification, spectral calibration, target spectrum extraction, and spectral alarming and matching.

HIPS is designed to operate on high-performance color workstations that use the X Window System™ and run under the UNIX™ operating system. Specifically, HIPS was developed on color Sun Microsystems SPARCstations™, and uses XView™ (X Window System-based Visual/Integrated Environment for Workstations) which is a user-interface toolkit to support interactive, graphics-based applications running under the X Window System.

HIPS provides the following functions:

- Versatile data input — ASCII or binary and BSQ, BIL, or BIP
- Image and image cube enhancement and display functions — 2-D and 3-D
- Spectra and vector display functions for data cube manipulation
- Calibration for image, sensor and atmospheric effects
- Convolution functions for transforming data from one source to the effective bands of another source; spatial and spectral filtering
- Basic mathematical operations, including algebraic and logical
- Supervised and unsupervised classification
- Resident spectrum library, including these features:
  - Other-source spectra can be added to library
  - Spectra from image cube can be extracted and added to library
  - Library spectra can be convolved to match image cube band passes
  - Search procedures for encoding and comparing library and image data sets
  - Spectrum feature identification procedures
- On-line help
- Interactive and batch processing modes
- Tools linked by an easy-to-use Graphical User Interface
- Functions are modular to facilitate changes and additions

The User Interface forms the interface between the user and the Computational Algorithms and will conform to the Open Look style guide using Sun's OpenWindow programming environment. This system is based on the X-Window System of windowing primitives, which is a de facto industry standard, and both offer network extensibility. Among other advantages, the use of such a graphical user interface (GUI) allows operation of the system from a remote bit-mapped workstation, with the remote user seeing exactly what a local user would see, but without actually running the software on the remote workstation. In a typical application, users will have a variety of windows open on their screen, containing color images, graphs of spectra, histograms, and other data, and command and input information and prompts.

The system will be built with four modes of user interaction, allowing the user to control the flow of data processing, i.e., procedure-based processing (PBP) in which a standard set of functions can be applied to a predictable or often repeated gas analysis scenario. An example scenario is described in Section III 1.1.6 Spatial Phenomena.

In **menu mode**, the user will be presented with a hierarchy of menus. Selection of a menu item will take the user either into another menu or into a function prompt screen, where parameters are entered for particular functions. The menu mode will be designed to "highlight" user specified default buttons to facilitate rapid progression from menu to menu, while providing the standard menu options in the event that a diversion in the processing chain is desired or necessary. In **command mode**, users can bypass the menu system and enter particular function prompt screens directly with a short (1–3) letter command. In **batch mode**, the user can fill out the parameters for a sequence of individual functions, and then submit the list of commands and parameters as a batch job, to be run in background. In **highly interactive mode**, a mouse and simple commands are available to control the visual display and the processing of data.

III.6 Conduct survey of existing data bases.

Spectrum libraries are available from many commercial and a few government and academic sources. Twelve of the organizations contacted provided information on gas spectrum libraries (see Table 4). With modifications, these can be accommodated by the HIPS™ Spectral Search Library for HyGAS™ operations. Additionally, HIPS™ provides the the option of extracting spectral data from the image data set being exploited for input into the Spectrum Search Library. This feature of HIPS™ enables the user to input "unknown spectra" for future analysis.

Table 4: Data Bases

Aldrich Chemical	IR libraries; FTIR libraries.
BOMEM, Inc.	IR libraries Environmental Protection Agency (EPA) vapor-based library, industrial).
EG&G	IR libraries.
Grumman Aerospace, Huntington	HCL & Methane gas; CO_2 & H_2O in smoke.
Infrared Analysis, Inc.	IR reference libraries (calibrated).
Lockheed Missiles & Space Co., Inc.	Vibration and rotation states of selected molecules.
Mattson Instruments, Inc.	FTIR libraries; GCIR libraries.

Table 4: Data Bases (cont.)

MIT	Gas spectrum libraries.
Nicolet	FTIR libraries; Vapor-phase library (with Aldrich).
Sadtler	IR libraries.
U.S. Army CRDEC	Gas data sets available upon official request.
University of Denver, Dept. of Chemistry	UV libraries.

Available data bases span the spectrum from the ultraviolet to the far-infrared. Some of the libraries contain spectral data which was measured in the gas or vapor phase (resulting in spectral line features), while others measured data using the liquid phase (resulting in spectral band features). Both types of data are appropriate for populating a spectral search library—the former for ultraspectral analysis and the latter for hyperspectral analysis. Information on several of these data bases has been archived at HyGAS™ contractor facility and is available for review.

We do not foresee any problems in designing a gas spectrum library interface to HIPS™. The acquisition and population of the gas spectrum libraries will be the responsibility of the sponsor or user of HyGAS™. The HyGAS™ contractor will provide the interface and a sufficiently basic gas library for proof of concept. The design of the gas spectral search library will provide the capability for additional spectra to be added and will be limited in size only by available disk space.

III.7 Design parallel processing interface.

Several excellent parallel processing systems in existence for several years are available and easily adaptable for integration into HIPS™ for the rapid, indeed realtime, processing of spectral and spatial data for gases. However, as improvements are made in multiprocessor technology, these capabilities are found incorporated within commercially available systems such as the 600 series SUNstations and Silicon Graphics systems. The processing capabilities of these systems approach the near realtime constraints of tactical decision making, i.e., minutes to accomplish spectral discrimination and alarming against a data base of candidates.

The overall system design defines that each of the computational algorithms be independent of the user interface and be standalone programs. This allows each of the computational algorithms to be developed and tested independently. Each of the individual programs will be divided into two primary types of modules: 1) I/O modules for data manipulations, and 2) computational routines for performing calculations on the data. Separating the program into individual modules allows the computation parts of the programs to access an on-line parallel processor and the I/O routines to operate on the front-end computer system.

The programs will go through several stages of development. During the first stage of development all of the programs will be written in C for fast prototyping and testing. Then, if the implementation is practicable, programs requiring higher through-put will be rewritten in C* , a parallel processing language version of C, to give access to an on-line parallel processor or to multi-processors in the case of a SUN 600 series computer or a Silicon Graphics. These routines could be tested on both a SUN 600 series computer and/or an on-line parallel processor which would be available starting in 1993.

The design of throughput of probabilistic information for gas detection and identification will be like that of the existing capability in HIPS™. The spectrum and interferogram matching algorithms will select several candidate matches and report a figure of merit for each candidate's "closeness of match".

III.8 Design integration of processing system and knowledge base.

HyGAS™ will contain all of the basic data base routines required for building and maintaining the Gas Spectral Library. In addition these routines will allow any of the modeling or search routines easy access to the data within the Gas Spectral Library. All of these will be incorporated into easy to use user interfaces which can be access in any of the operational modes of HyGAS™.

IV. Conclusions

The conclusions of the HyGAS™ team in reviewing the information gathered are:

- The technical and scientific requirements for spectral processing of gas spectra are historical; systems for the acquisition, detection, and analysis of gases have been in use for many decades. Refinements to these are continuous and include Fourier transform infrared spectroscopy, the use of interferogram techniques, and the application of imaging spectrometers to acquire gas spectra, adding the spatial dimension; HyGAS™ can accommodate these techniques.

- Spectral processing software has been in use for many decades and spatial processing software for several decades. Spectral matching and Fourier transform analysis are common categories with the recent addition of interferogram processing. The former two are widely available, however, sometimes in specialized form and for use with specialized spectral processing equipment. There is no processing system known to us which incorporates both of these categories of processing into a consolidated unit; HyGAS™ will do so.

- The HyGAS™ study has shown that the Hyperspectral Image Processing System (HIPS™), developed under an SBIR contract with the U.S. Army, Topographic Engineering Center, Ft. Belvoir, Va., COTR, Mr. Sam Barr, to be easily adapted to use for analysis of hyperspectral and ultraspectral gas spectral data. Gas analysis functions can be developed and integrated into HIPS™ for HyGAS™.

- HIPS™ presently incorporates spectral search of a data set (image cube) against a spectrum library. Spectral matching routines retrieve candidates from the list of available spectra with probability constraints on the selections. Fourier transform and interferogram analysis algorithms are easily added to the HIPS™ library of processing functions.

- Many excellent instruments for the detection and identification of gases have been and are in use in the laboratory and in the field of which point detection systems are by far the most common. Far fewer imaging spectrometers are available and are primarily hyperspectral systems. Thus, gas spectral imagery could be acquired.

- Designs for imaging hyperspectral sensors (gas band versus line discrimination) are available which meet the specifications for gas detection, SNR greater than 300:1 at a 0.05 albedo, a NESR of 0.01, a NEΔT of 0.1 K, and $\Delta\lambda/\lambda$ of 0.01. The limiting factor is the insufficient detector technology in fabricating large detector arrays for the mid- and far infrared regions so critical to gas detection. (See Table 3.)

- Spectrum libraries are available from many commercial (proprietary) and a few government and academic sources (see Table 4). With modifications, these can be accommodated by the HIPS™ Spectral Search Library for HyGAS™ operations. Additionally, HIPS™ provides the the option of extracting spectral data from the image being exploited for input into the Spectrum Search Library. This feature of HIPS™ enables the user to input "unknown spectra" for future analysis and will be designed into HyGAS™.

- Several excellent parallel processing systems are available and easily adapted for integration into the HIPS™ for the rapid, realtime, processing of spectral and spatial data for gases. However, as improvements are made in multiprocessor technology, these capabilities are found incorporated within commercially available systems such as the 600 series SUNstations and Silicon Graphics systems. The processing capabilities of these systems approach the near real time constraints of tactical decision making, i.e., minutes to accomplish spectral discrimination and alarming against a data base of candidates. Either technology is applicable to HyGAS™.

V. Estimates of Technical Feasibility

No technical problems have been identified that would prevent the implementation of the defined system under Phase II. However, it should be noted that the degree to which certain processing algorithms work, such as atmospheric correction, will be strongly affected by the data sets used (i.e. wavelength range, signal-to-noise ratio, and calibration).

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